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*Physics Department, Cleveland State University¹⁾***Cohesive Energy–Lattice Constant Relationship**

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Recently [1], we showed that for the alkali, Ag, and Tl halides, the product of the cohesive energy, E_{coh} , with the equilibrium nearest neighbor distance, d_{nn} , is to a good approximation constant within families of solids with common crystal structure. In this note we demonstrate that this relationship holds for several other families of solids in their low pressure phases. These include: group II chalcogenides and halides, alkali hydrides, ammonium halides, alkali chalcogenides, and iron group transition metal oxides.

The numerical values of $E_{\text{coh}}d_{\text{nn}}$ for the individual solids within each family with common crystal structure are listed in Table 1. The sources for the values of E_{coh} and d_{nn} used are also tabulated. In Table 2 the average value of $E_{\text{coh}}d_{\text{nn}}$ within each group is listed along with the RMS deviation. Note that the RMS deviation varies from 0.19% to a maximum of 2.70% for the transition metal and group II oxides. Thus we may conclude that to a very good approximation the product $E_{\text{coh}}d_{\text{nn}}$ is constant within families of solids with common crystal structure.

Table 1
Values of $E_{\text{coh}}d_{\text{nn}}$

solid	E_{coh} (kcal/mol)	d_{nn} (Å)	$E_{\text{coh}}d_{\text{nn}}$ (kcal Å/mol)	crystal structure	references	
					E_{coh}	d_{nn}
MgO	932	2.105	1962	NaCl	a	b
CaO	839	2.405	2018	NaCl	a	b
SrO	796	2.580	2054	NaCl	a	b
BaO	786	2.761	2170	NaCl	a	b
MnO	910.9	2.222	2024	NaCl	c	b
FeO	938.4	2.155	2022	NaCl	c	b
CoO	954.6	2.133	2036	NaCl	c	b
NiO	975.4	2.084	2033	NaCl	c	b
MgS	800	2.602	2081	NaCl	a	d
CaS	764	2.845	2173	NaCl	a	d
SrS	720	3.010	2167	NaCl	a	d
BaS	679	3.194	2169	NaCl	a	d
MgSe	798	2.731	2179	NaCl	a	d
CaSe	726	2.960	2149	NaCl	a	d
SrSe	693	3.120	2162	NaCl	a	d
BaSe	660	3.300	2178	NaCl	a	d
CaTe	679	3.179	2158	NaCl	a	a
SrTe	667	3.331	2222	NaCl	a	a

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Table 1 (continued)

solid	E_{coh} (kcal/mol)	d_{nn} (Å)	$E_{\text{coh}}d_{\text{nn}}$ (kcal Å/mol)	crystal structure	references	
					E_{coh}	d_{nn}
BaTe	629	3.500	2202	NaCl	a	a
NaH	192.5	2.44	469.7	NaCl	d	d
KH	170.0	2.83	481.1	NaCl	d	d
RbH	162.9	3.02	492.0	NaCl	d	d
CsH	155.8	3.19	497.0	NaCl	d	d
NH ₄ Cl	170.0	3.348	569.1	CsCl	d	d
NH ₄ Br	162.9	3.505	570.1	CsCl	d	d
NH ₄ I	151.6	3.784	573.7	CsCl	d	d
CaF ₂	629.8	2.36	1486	CaF ₂	d	d
SrF ₂	596.7	2.51	1498	CaF ₂	d	d
BaF ₂	563.3	2.68	1510	CaF ₂	d	d
SrCl ₂	514.7	3.02	1554	CaF ₂	d	d
BaCl ₂	490.6	3.18	1560	CaF ₂	d	d
Li ₂ O	685.7	2.000	1371	α	e	d
Li ₂ S	569.8	2.472	1409	α	e	d
Li ₂ Se	535.9	2.600	1393	α	e	d
Li ₂ Te	505.8	2.820	1426	α	e	d
Na ₂ O	590.6	2.403	1419	α	e	d
Na ₂ S	504.4	2.826	1425	α	e	d
Na ₂ Se	475.9	2.948	1403	α	e	d
Na ₂ Te	452.0	3.17	1432	α	e	e
K ₂ O	543.8	2.787	1516	α	e	d
K ₂ S	458.8	3.200	1468	α	e	d
K ₂ Se	433.8	3.324	1442	α	e	d
K ₂ Te	413.0	3.54	1462	α	e	e
Rb ₂ O	539.3	2.919	1574	α	e	d
Rb ₂ S	450.7	3.313	1493	α	e	d

structure: α means antiferite

references: a [2], b [3], c [4], d [5], e [6]

Table 2

Average values of $E_{\text{coh}}d_{\text{nn}}$

	$E_{\text{coh}}d_{\text{nn}}$ (kcal Å/mol)	RMS deviation (%)	crystal structure
transition metal oxides, group II oxides	2040 ± 55.1	2.70	NaCl
group II sulphides, selenides, tellurides	2167 ± 33.4	1.54	NaCl
alkali hydrides	485.0 ± 10.5	2.17	NaCl
ammonium halides	571.3 ± 1.89	0.33	CsCl
group II fluorides	1498 ± 9.80	0.65	CaF ₂
group II chlorides	1557 ± 3.00	0.19	CaF ₂
lithium and sodium chalcogenides	1410 ± 19.1	1.35	α
potassium chalcogenides	1472 ± 27.2	1.85	α
rubidium chalcogenides	1534 ± 40.5	2.64	α

structure: α means antiferite

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